Testing of the June 2002 Version of the United States EPA's CMAQ

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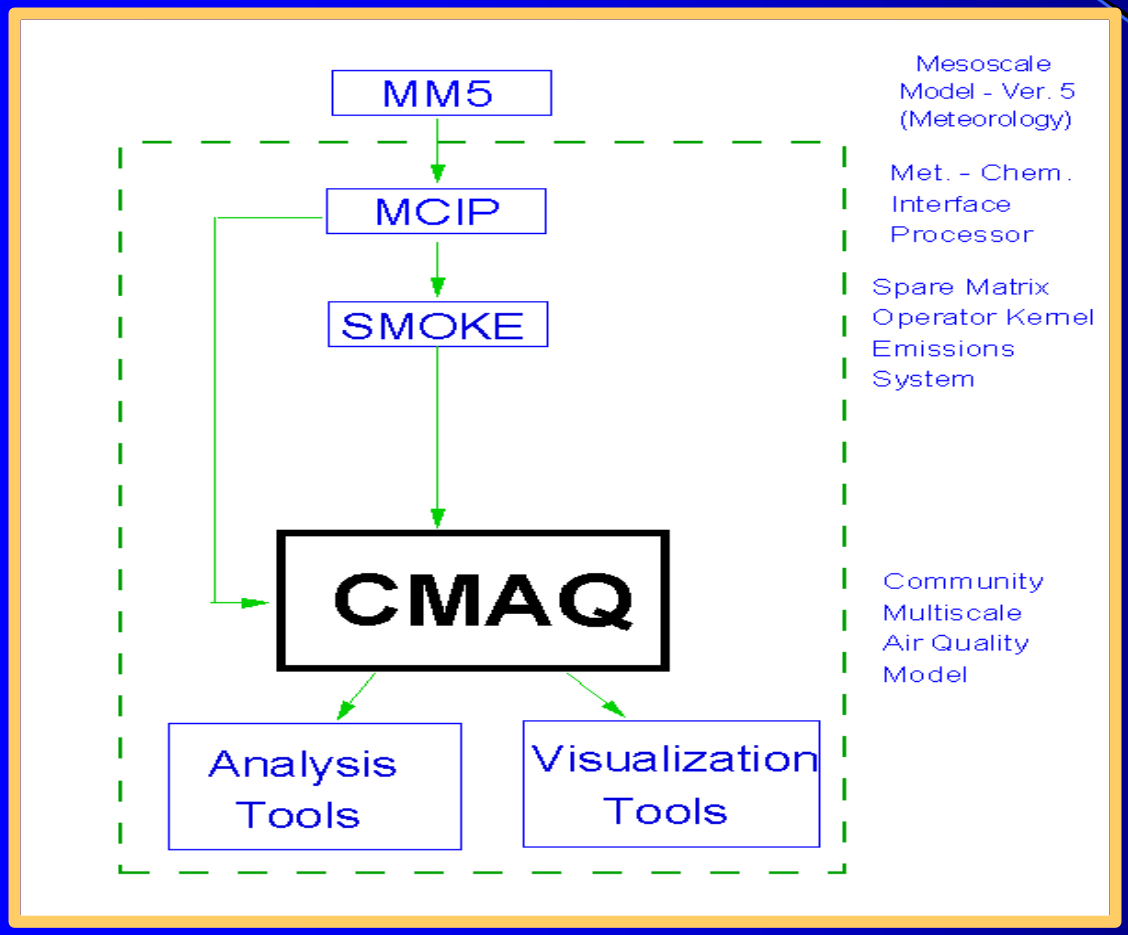
Models – 3 Framework



CMAQ Community Multiscale Air Quality Model

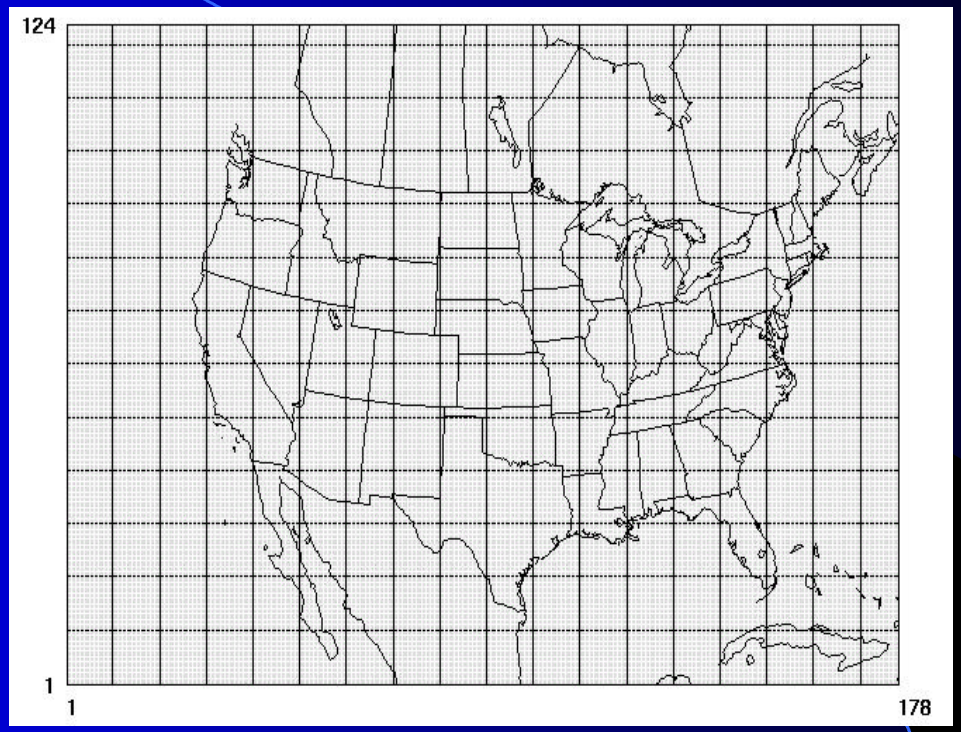
- **Community Model**
- **Multiscale**
  - consistent model structures for interaction of *urban* through *Continental* scales
- **Multi-pollutant**
  - ozone, speciated particulate matter, visibility, acid deposition and air toxics

CMAQ

- New “Base” Configuration
  - SAPRC99 gas-phase chemistry
  - AE3 aerosol module
  - BEIS 3.09 biogenic emissions

Spatial Domain

- 32 km grid resolution
- 22,072 grid cells



Temporal Domain

- 1- 14 July, 1999

Species, Metrics and Networks

O_3	Hourly, max 1-hr, max 8-hr (**AIRS**)
SO_2	Mean weekly (**CASTNet**)
SO_4	Mean weekly (**CASTNet**), Mean 24-hr (**IMPROVE**)
NO_3	Mean weekly (**CASTNet**), Mean 24-hr (**IMPROVE**)
HNO_3	Mean weekly (**CASTNet**)
$PM_{2.5}$	Mean 24-hr (**IMPROVE**)
OMC	Mean 24-hr (**IMPROVE**)
EC	Mean 24-hr (**IMPROVE**)
NH_4	Mean weekly (**CASTNet**)

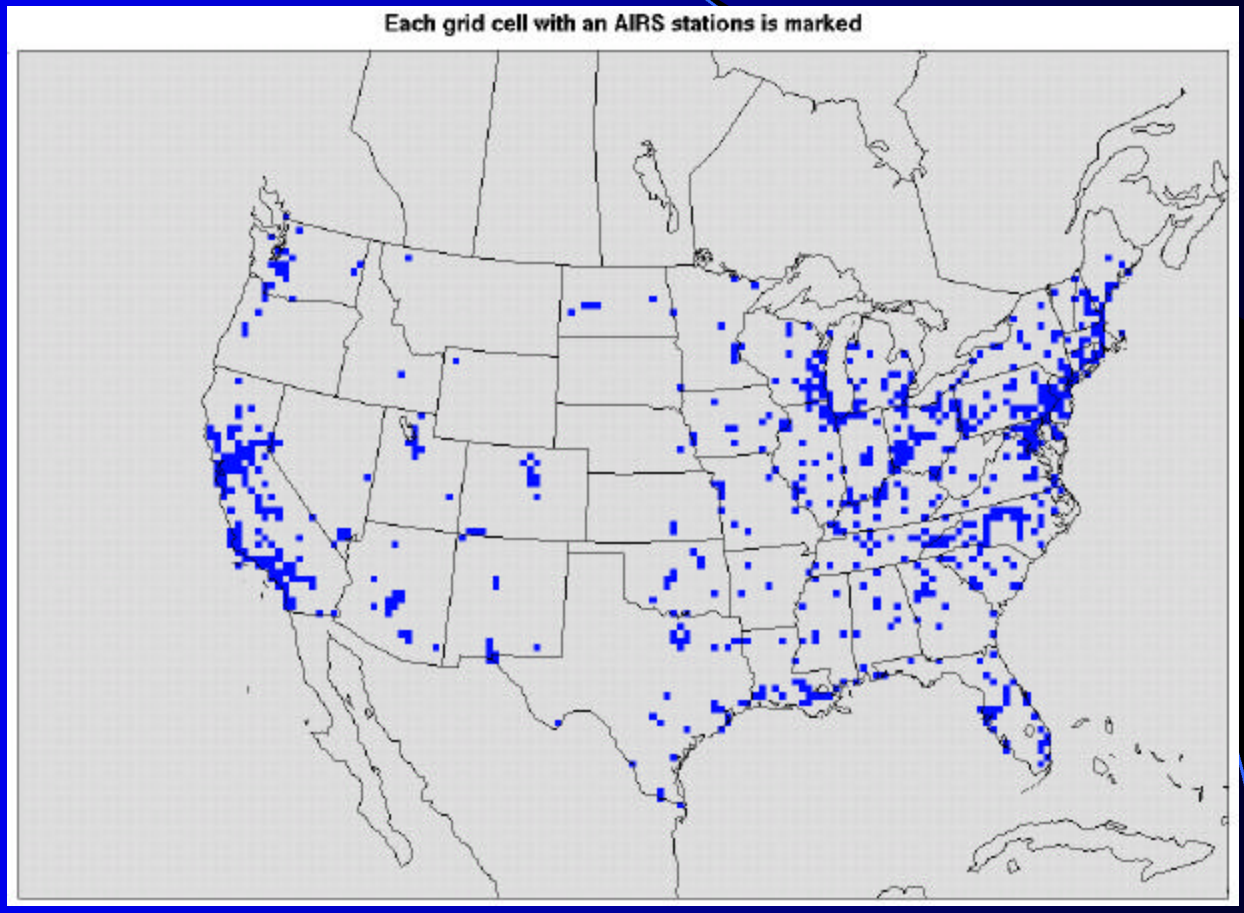
AIRS

Aerometric **I**nformation **R**etrieval **S**ystem

Hourly data for each of the 14 days

1,032 Stations
234,384 Obs

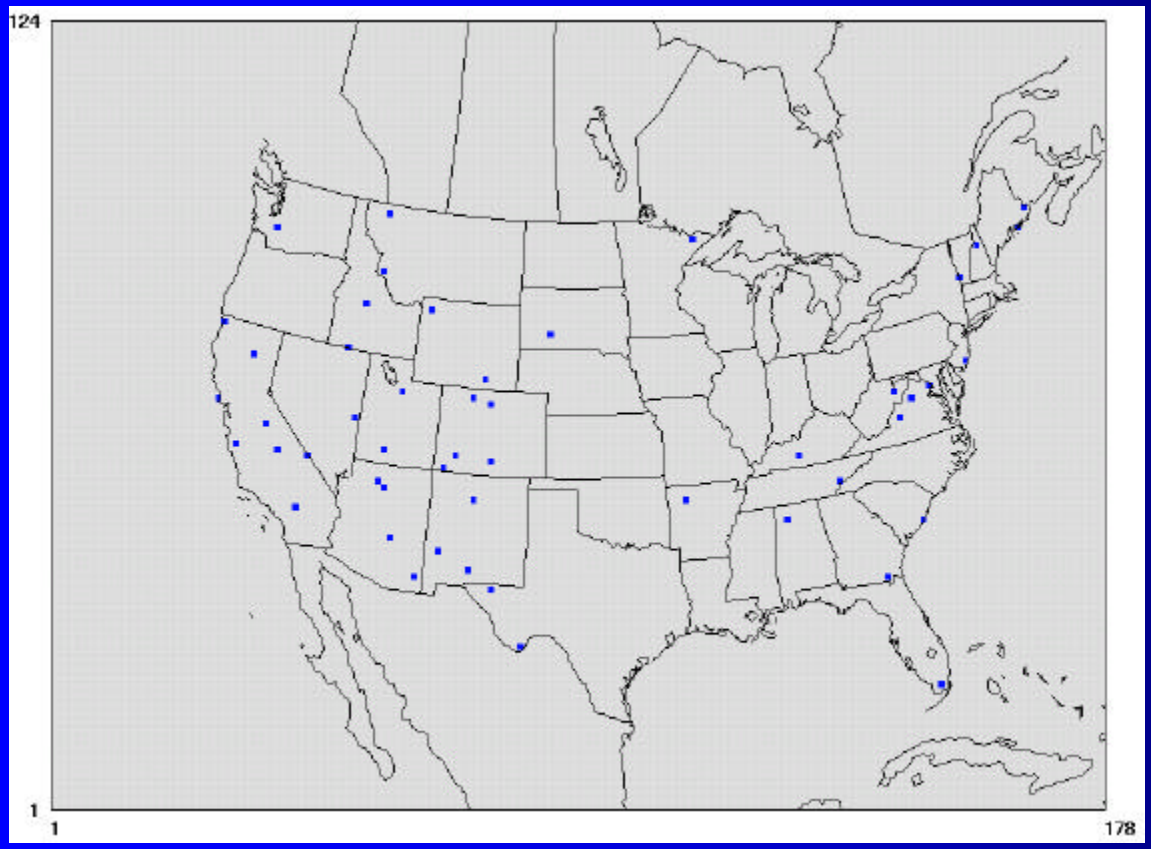
O_3



IMPROVE Interagency Monitoring of PROtected Visual Environments

24-hr means for: 3, 7, 10, 14 July

50 Stations
200 Observations



SO_4

NO_3

$PM_{2.5}$

OMC

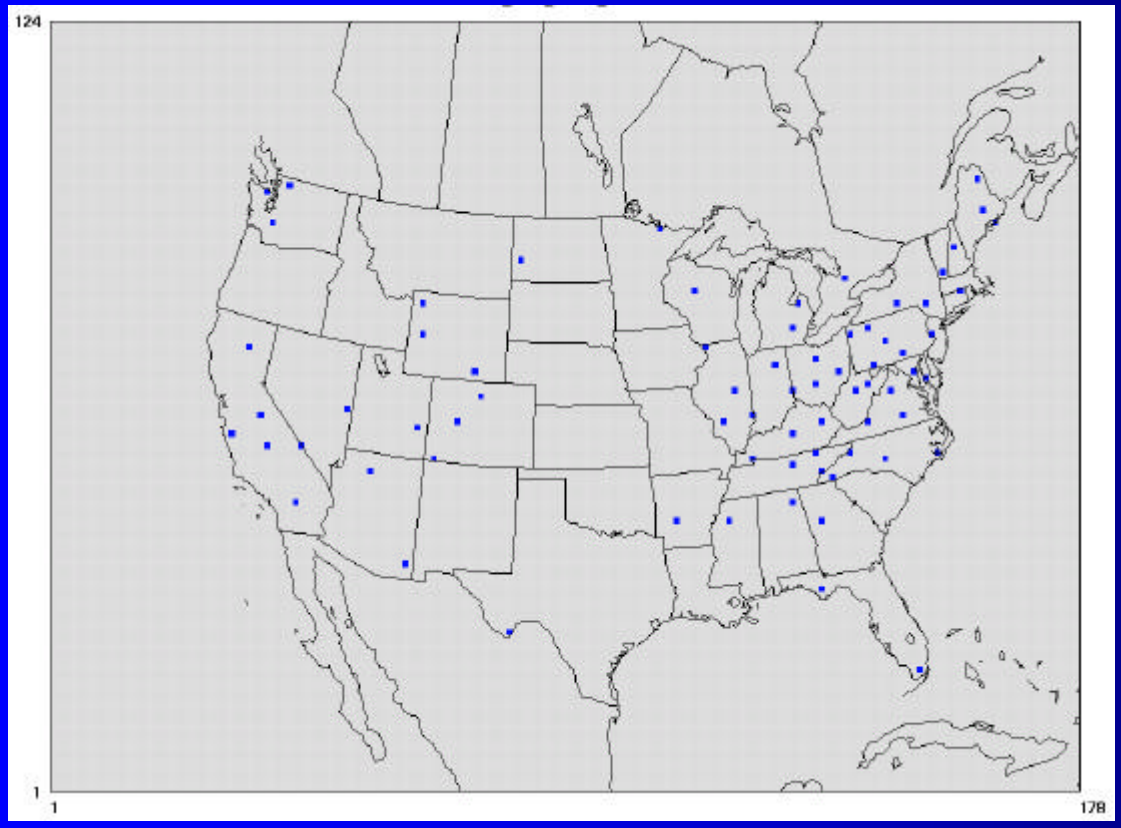
EC

CASTNet

Clean Air Status and Trends Network

Weekly means for 6 –13 July

59 Stations,
59 Observations



SO_2

SO_4

HNO_3

NH_4

Statistics - Errors

Normalized Mean Error

$$NME = \frac{\sum_{1}^{N} |Model - Obs|}{\sum_{1}^{N} (Obs)} \cdot 100\%$$

Root Mean Square Error

$$RMSE = \frac{1}{N} \sum_{1}^{N} (Model - Obs)^2$$

Mean Absolute Gross Error

$$MAGE = \frac{1}{N} \sum |Model - Obs|$$

Mean Normalized Gross Error

$$MNGE = \frac{1}{N} \sum_{1}^{N} \left(\frac{|Model - Obs|}{Obs} \right) \cdot 100\%$$

Statistics - Biases

Mean Bias

$$MB = \frac{1}{N}\sum_{1}^{N}(Model - Obs)$$

Mean Normalized Bias

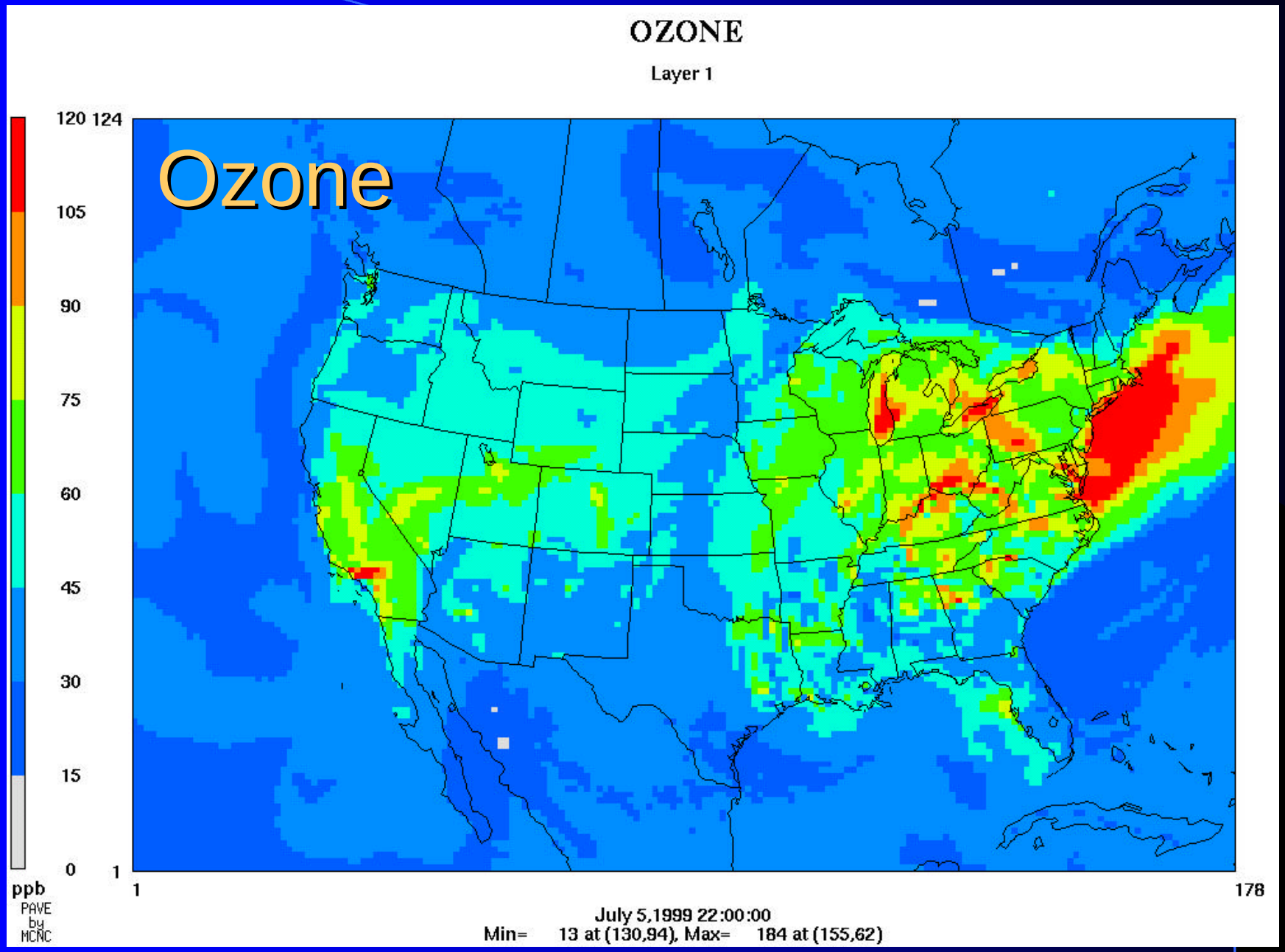
$$MNB = \frac{1}{N}\sum_{1}^{N}\left(\frac{(Model - Obs}{Obs}\right)\cdot 100\%$$

Mean Fractionalized Bias

$$MFB = \frac{1}{N}\sum_{1}^{N}\left(\frac{(Model - Obs)}{\left(\frac{Model + Obs}{2}\right)}\right)\cdot 100\%$$

Normalized Mean Bias

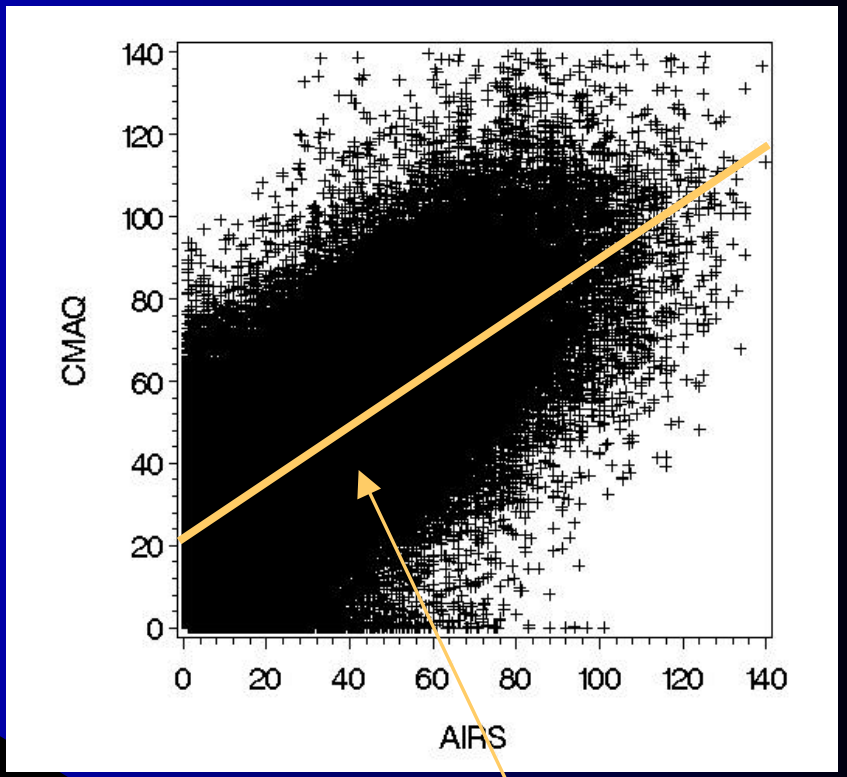
$$NMB = \frac{\sum_{1}^{N}(Model - Obs)}{\sum_{1}^{N}(Obs)}\cdot 100\%$$


OZONE
Layer 1
Ozone
120 124
105
90
75
60
45
30
15
0
ppb
PAVE
by
MCNC
1
1
178
July 5,1999 22:00:00
Min= 13 at (130,94), Max= 184 at (155,62)

Ozone

- Hourly

	CMAQ	OBS		
Mean	45.4	34.6	n	234,384
SD	20.2	20.1	R	0.68
CV	44.5%	58.2%	MB	10.8
Max	203.2	155.0	MNB	111.0%
95th	81.0	71.0	MFB	31.4%
75th	57.7	47.0	MAGE	15.2
50th	43.6	32.0	MNGE	122.4%
25th	31.6	20.0	NME	31.4%
5th	15.4	6.0	NMB	23.7%
Min	0.0	1.0	RMSE	19.5



CMAQ = 22.0 + 0.68 OBS

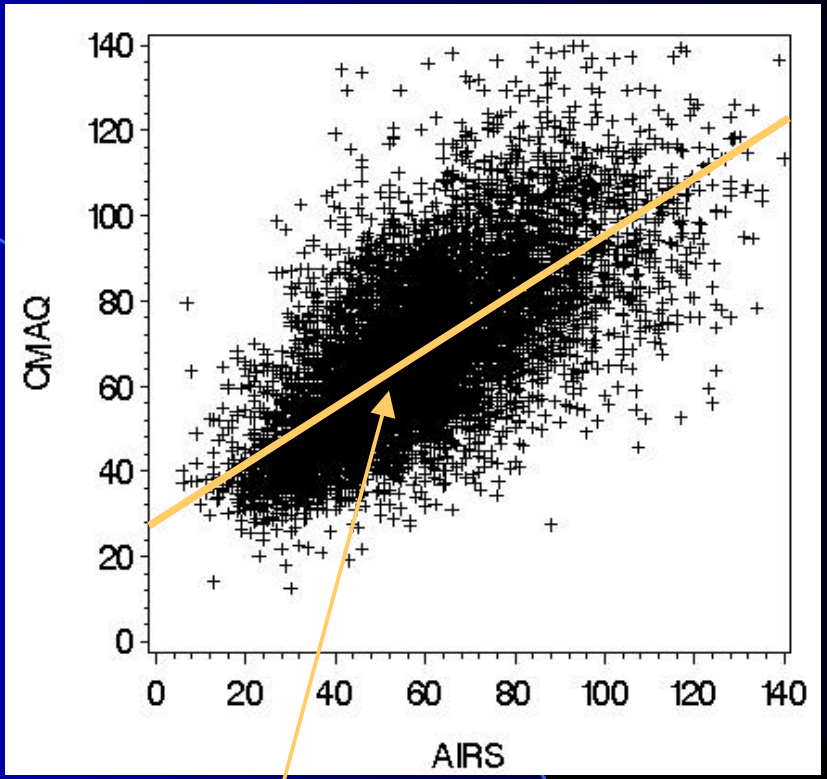
CMAQ Performance

- Biases positive and generally small
- MNB, MNGE inflated due to small hourly obs.

Ozone

- Max 1-hr

	CMAQ	OBS		
Mean	67.3	58.1	n	10,149
SD	20.0	20.5	R	0.71
CV	29.7%	35.2%	MB	9.2
Max	203.2	155.0	MNB	22.7%
95th	102.7	95.0	MFB	16.4%
75th	79.9	71.0	MAGE	14.0
50th	65.5	56.0	MNGE	29.0%
25th	52.6	44.0	NME	24.0%
5th	38.7	28.0	NMB	15.8%
Min	12.6	6.0	RMSE	18.0



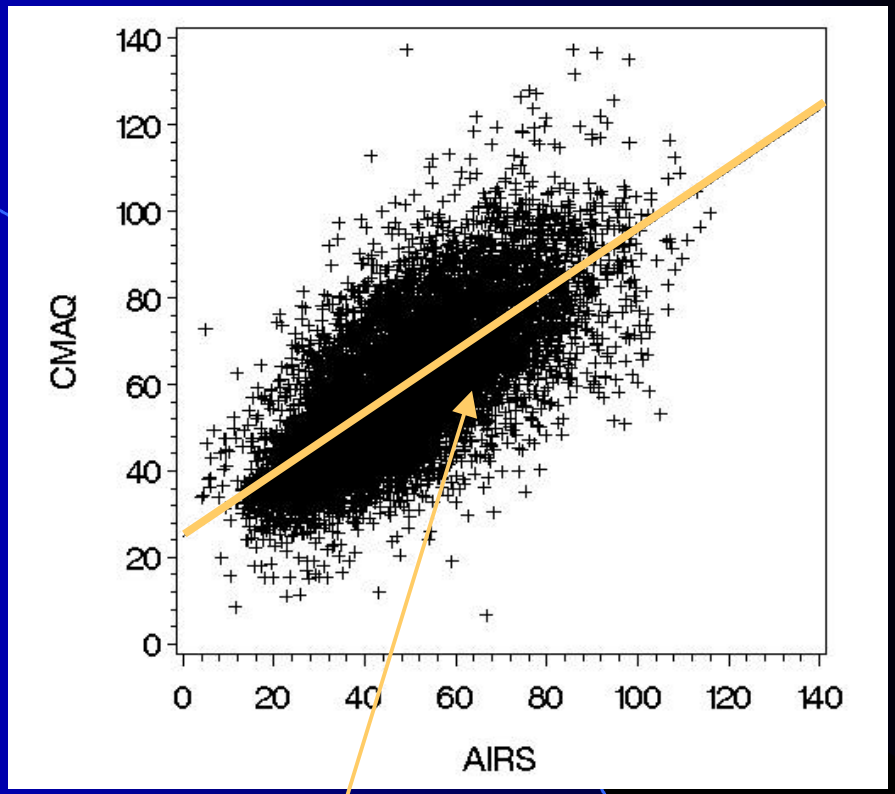
CMAQ = 28.0 + 0.67 OBS

CMAQ Performance

- Biases smaller, still positive
- Errors smaller
- MNB, MNGE closer to other statistics

Ozone

- Max 8-Hr



CMAQ = 24.7 + 0.71 OBS

	CMAQ	OBS		
Mean	59.4	49.0	n	10,149
SD	17.0	17.2	R	0.72
CV	28.7%	35.1%	MB	10.4
Max	168.3	116.0	MNB	29.1%
95th	88.6	79.8	MFB	21.1%
75th	70.8	60.0	MAGE	13.2
50th	58.0	47.6	MNGE	33.6%
25th	46.7	36.3	NME	26.9%
5th	34.8	23.4	NMB	21.2%
Min	6.7	4.2	RMSE	16.5

CMAQ Performance

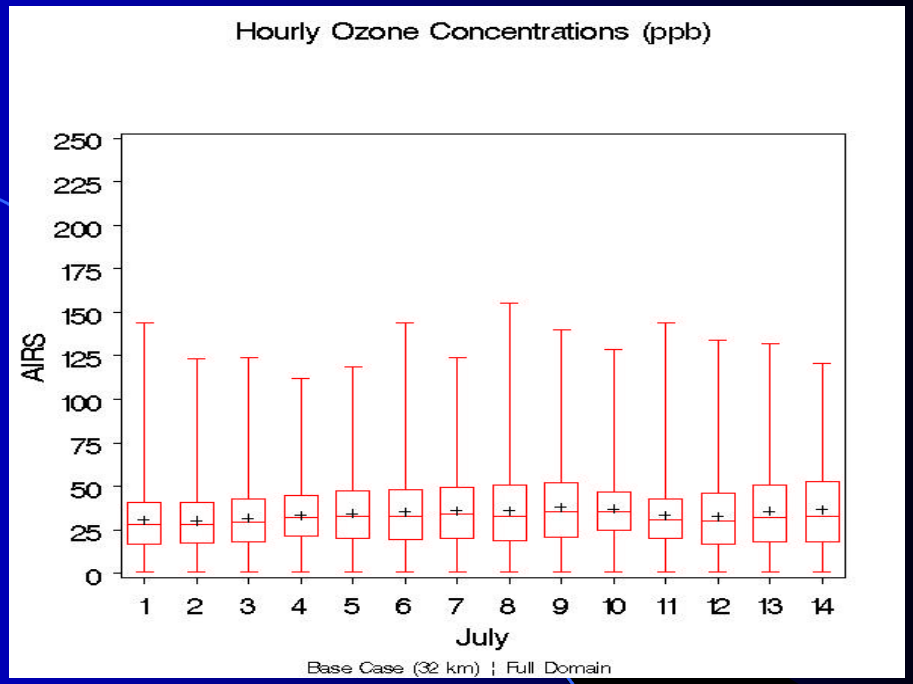
- Biases positive, smaller than hourly, larger than max 1-hr
- Errors generally smaller

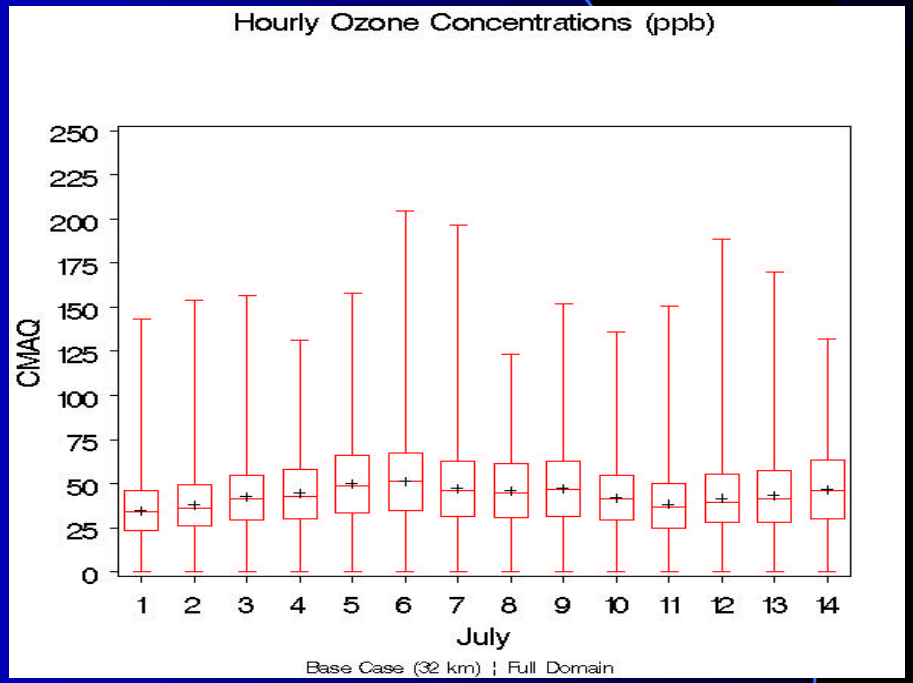
Daily Boxplots

- Ozone
  - Hourly

Observations increase from 1–9 July, then decreases from 10 -12, then increase thru 14.

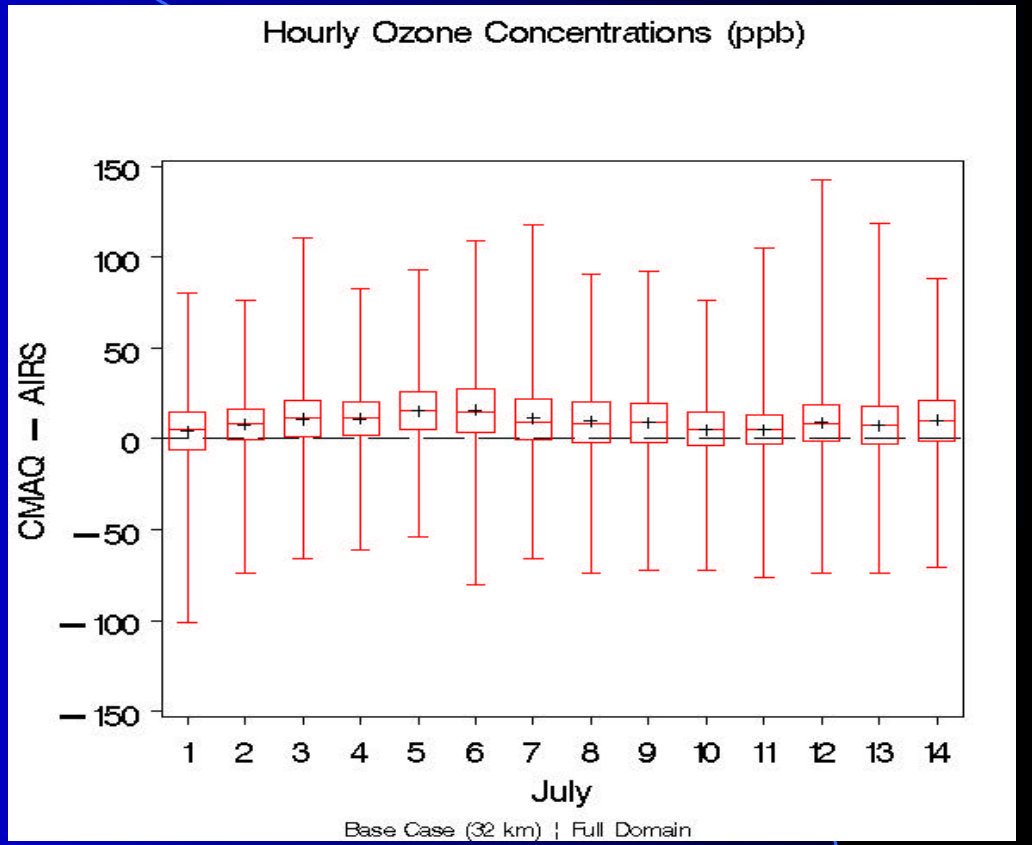
Simulations increase from 1–6 July, decrease on 7 and again on the 10 and 11, then increase thru 14.





Daily Boxplots

- Ozone Difference
  - Hourly
  - CMAQ - AIRS



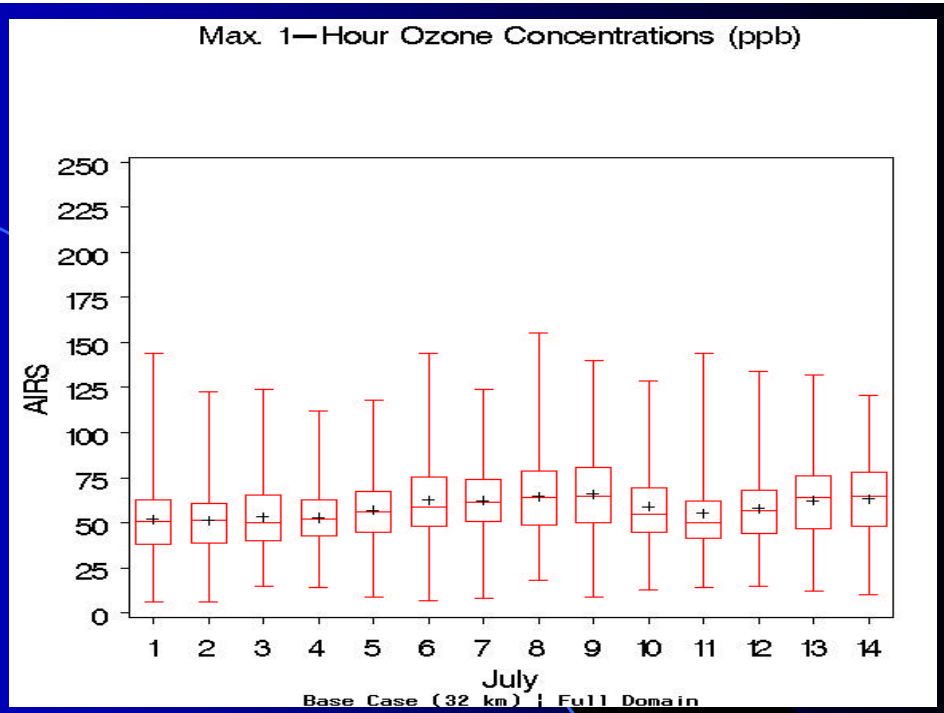
Biases are positive on all days.

Largest biases occur on 5 and 6 July

Smallest occur on 1, 10 and 11 July

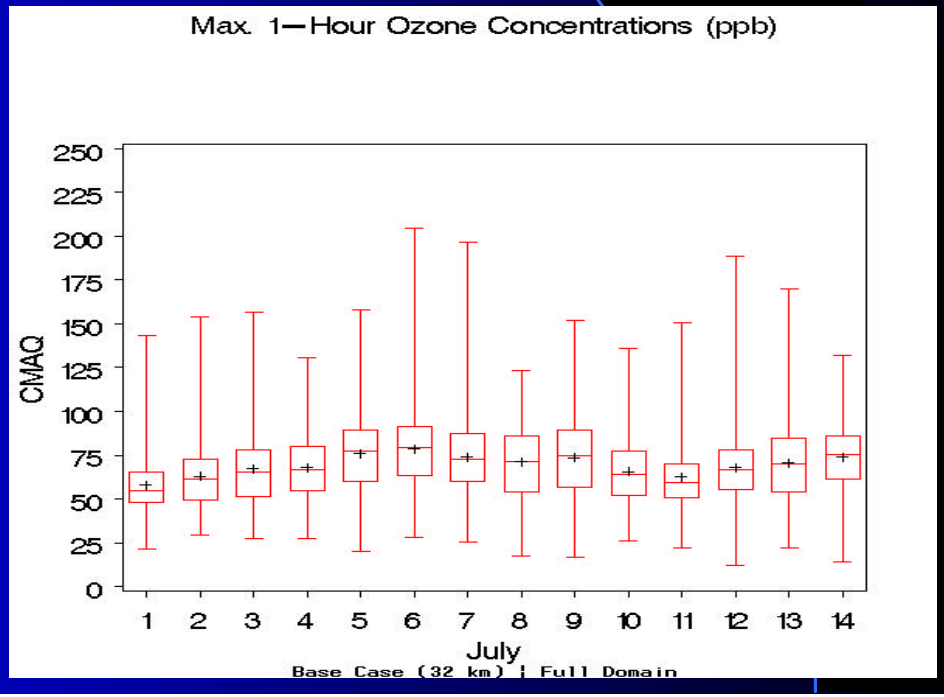
Daily Boxplots

- Ozone
  - Max 1-Hr



Observations increase from 1–8 July, then decreases from 10 -11, then increase thru 14.

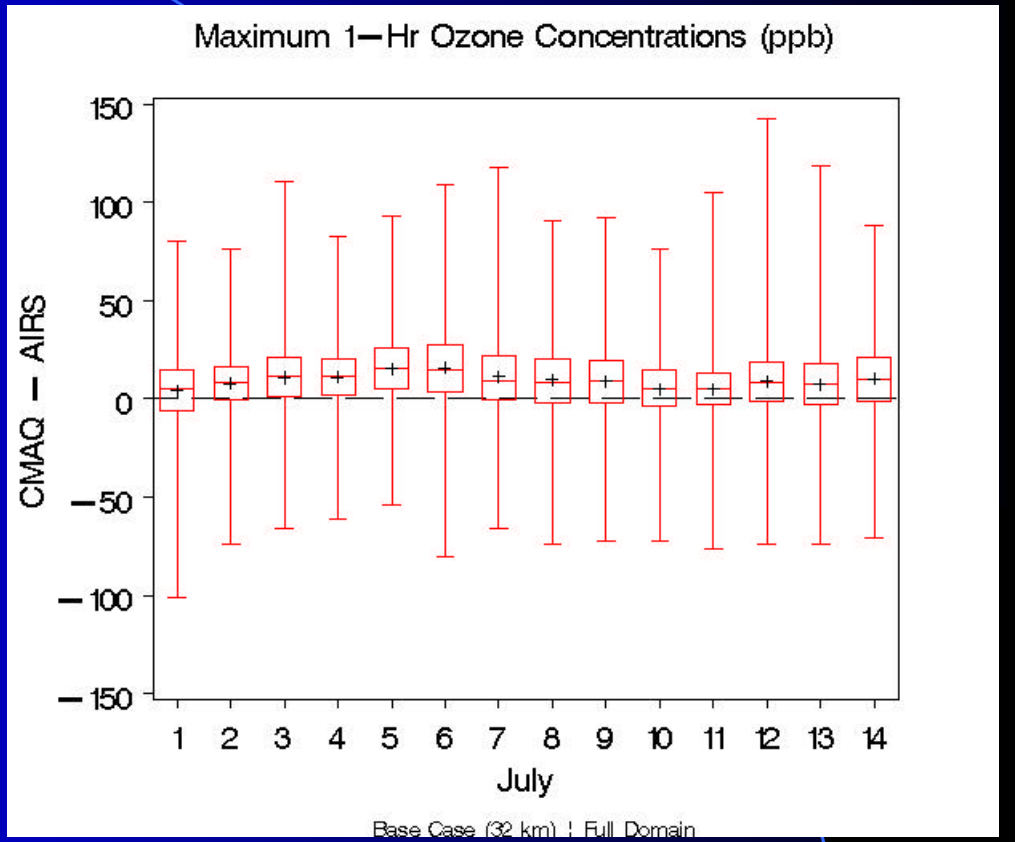
Simulations increase from 1–6 July, decrease on 7 and again on the 10 and 11, then increase thru 14.



Daily Boxplots

- Ozone Differences

  - Max 1-Hr
  - CMAQ - AIRS



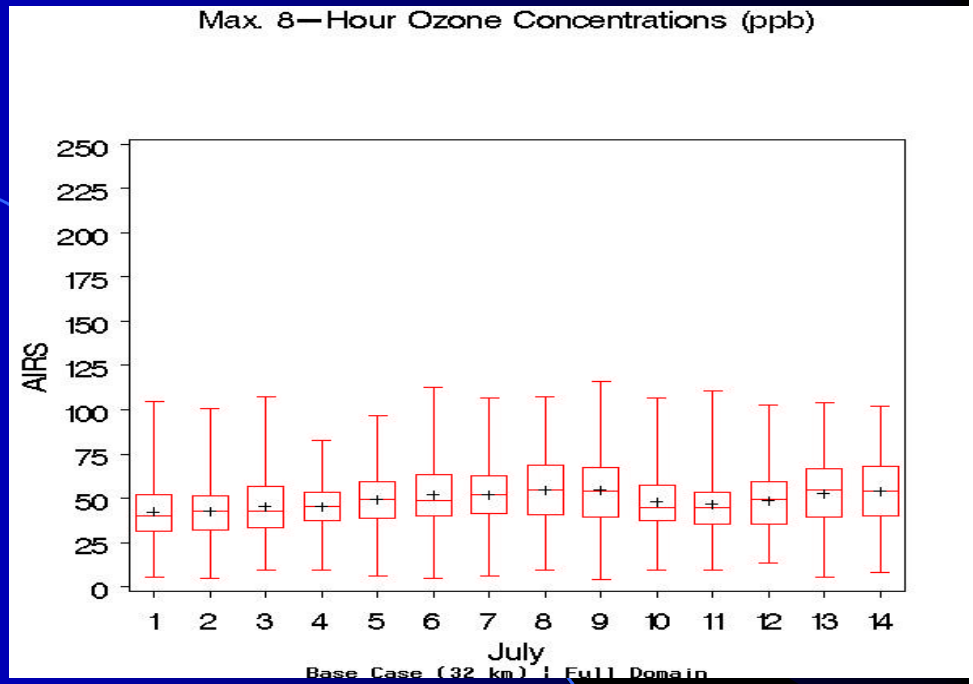
Biases are again positive on all days.

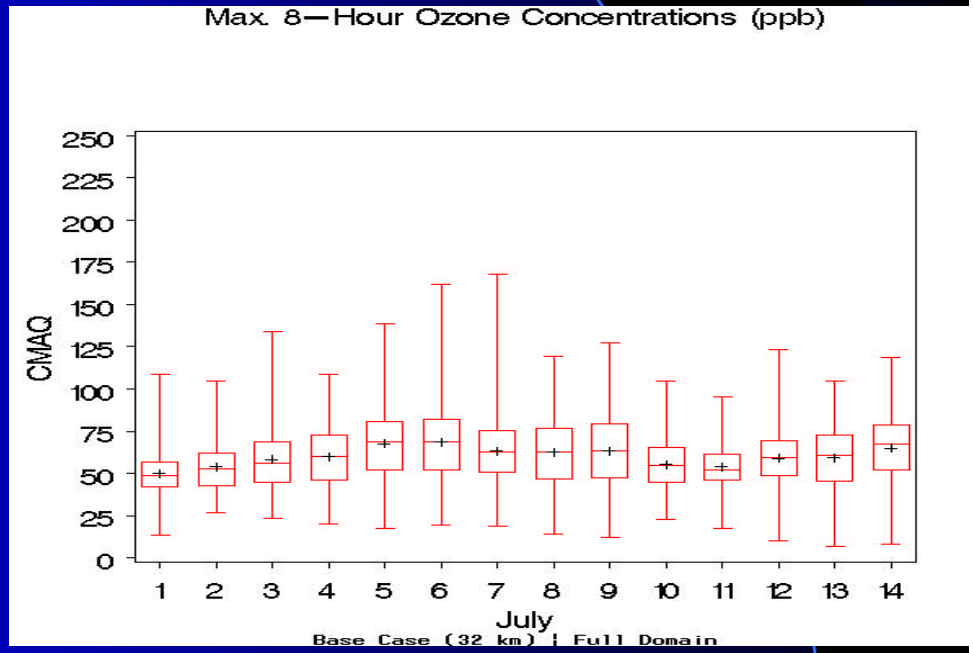
Largest biases occur on 5 and 6 July

Smallest occur on 1, 10 and 11 July

Daily Boxplots

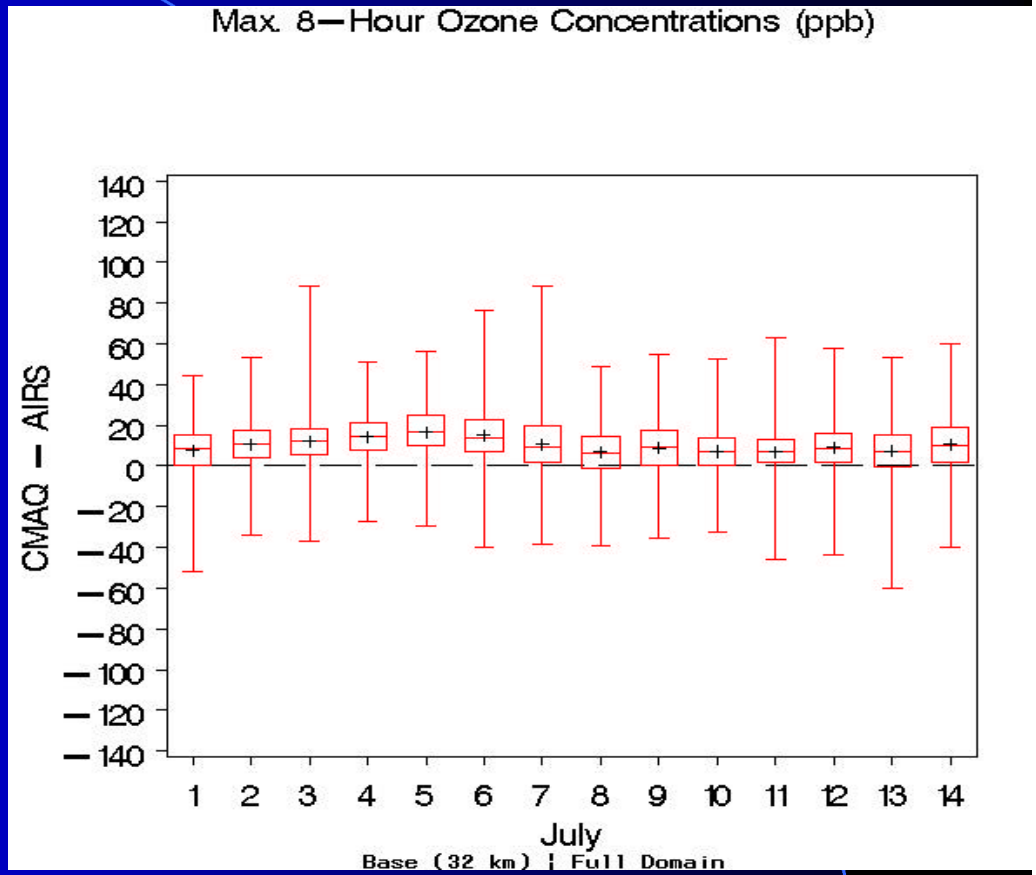
- Ozone
  - Max 8-Hr





Daily Boxplots

- Ozone
  - Max 8-Hr
  - CMAQ - AIRS

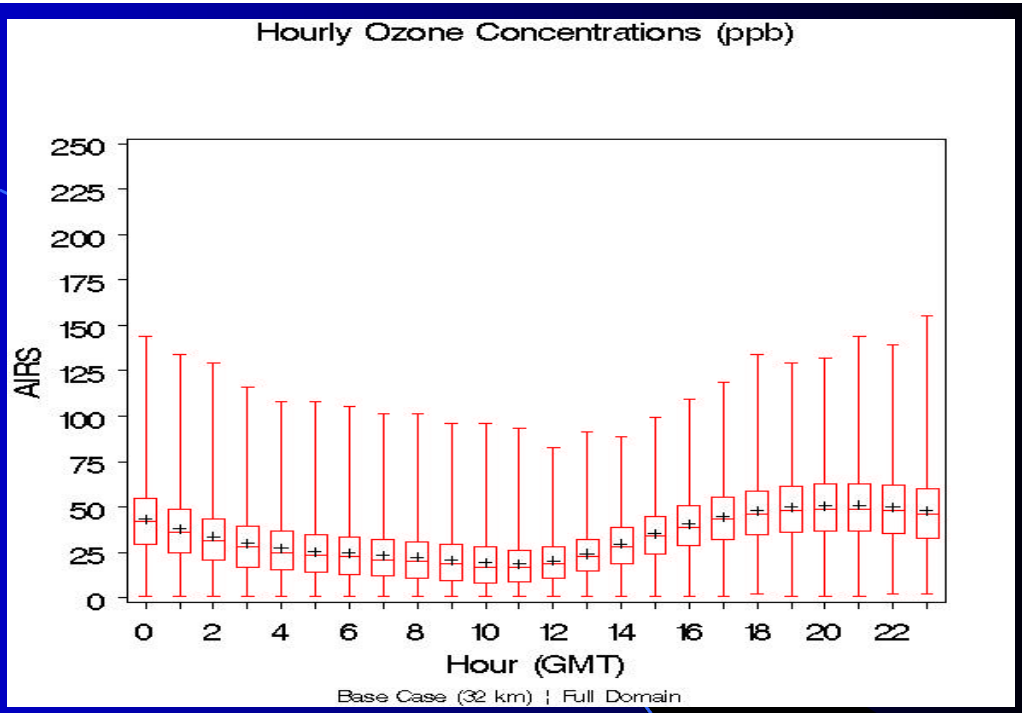


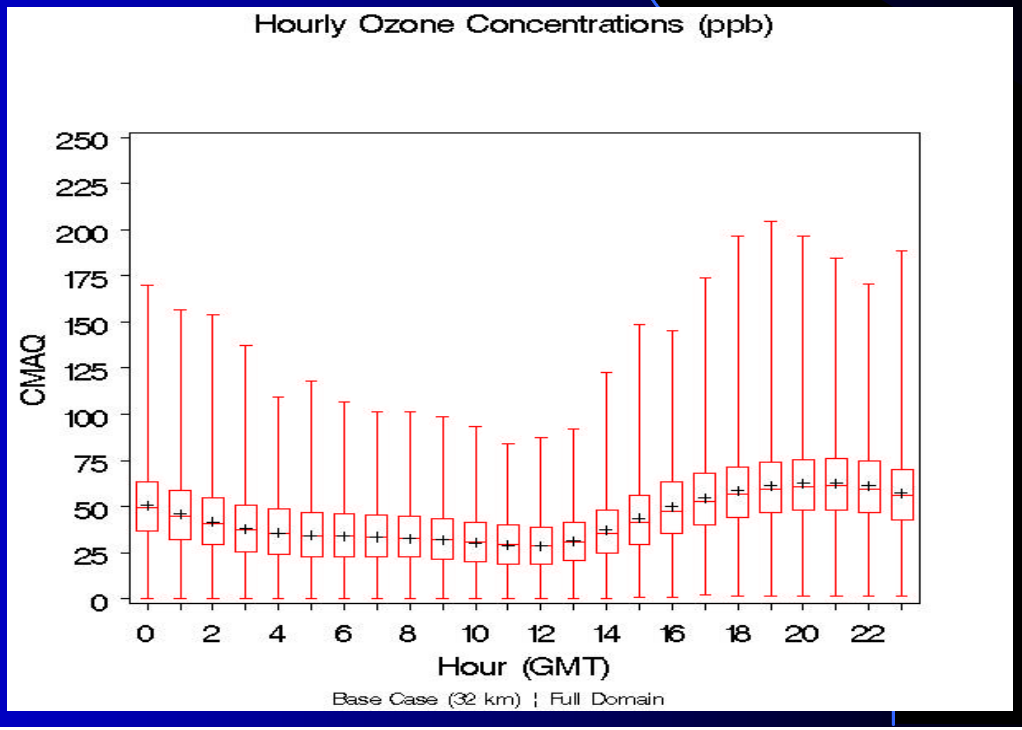
Hourly Boxplots

- Ozone

Diurnal pattern is well replicated by the model

- morning minimum (11 - 12 GMT)
- afternoon maximum (20 - 21 GMT)



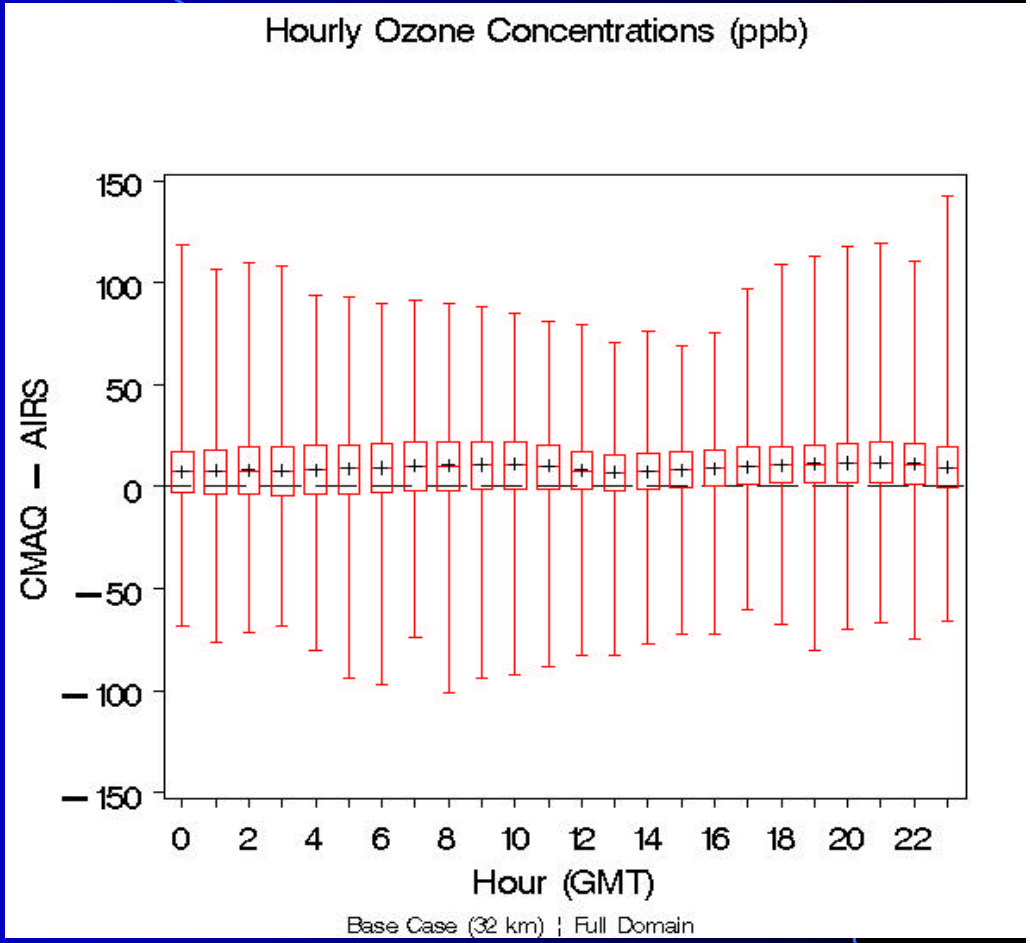


Hourly Boxplots

- Ozone

CMAQ - AIRS

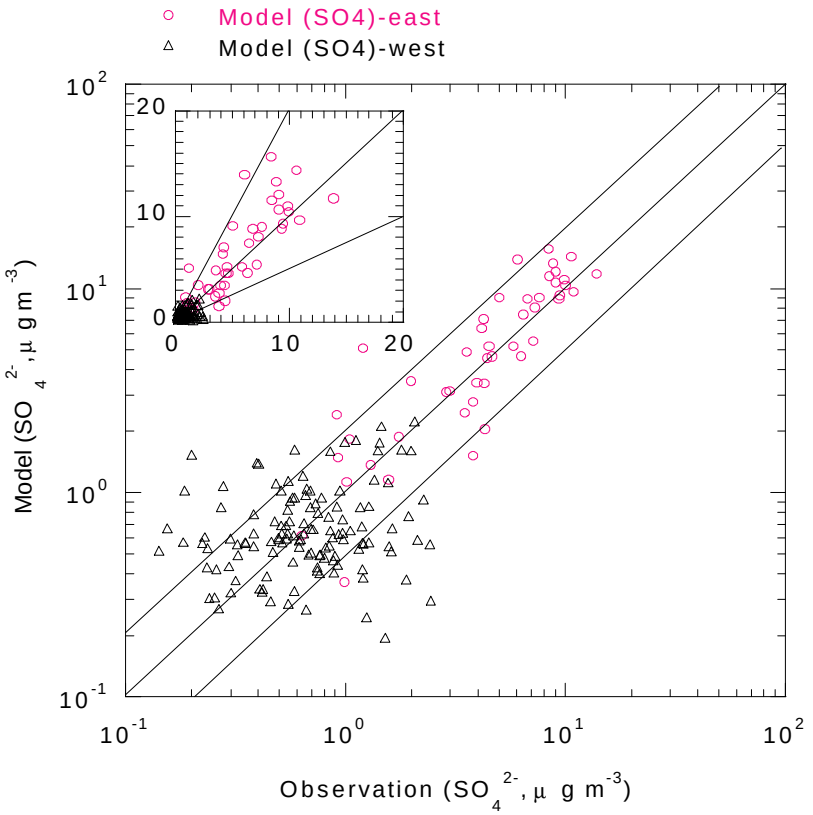
- Biases are always positive
- Biases smallest in pm when atmosphere is well mixed.



SO_4

- 24-Hr mean
- IMPROVE

	CMAQ	OBS	CMAQ = -0.07 + 1.13 OBS	
Mean	2.18	1.99	n	174
SD	3.27	2.66	R	0.92
CV	149.8%	133.8%	MB	0.19
Max	15.60	13.88	MNB	32.6%
95th	10.70	9.04	MFB	2.1%
75th	1.76	1.89	MAGE	0.73
50th	0.72	0.86	MNGE	61.0%
25th	0.54	0.54	NME	36.8%
5th	0.31	0.24	NMB	9.5%
Min	0.19	0.14	RMSE	1.31

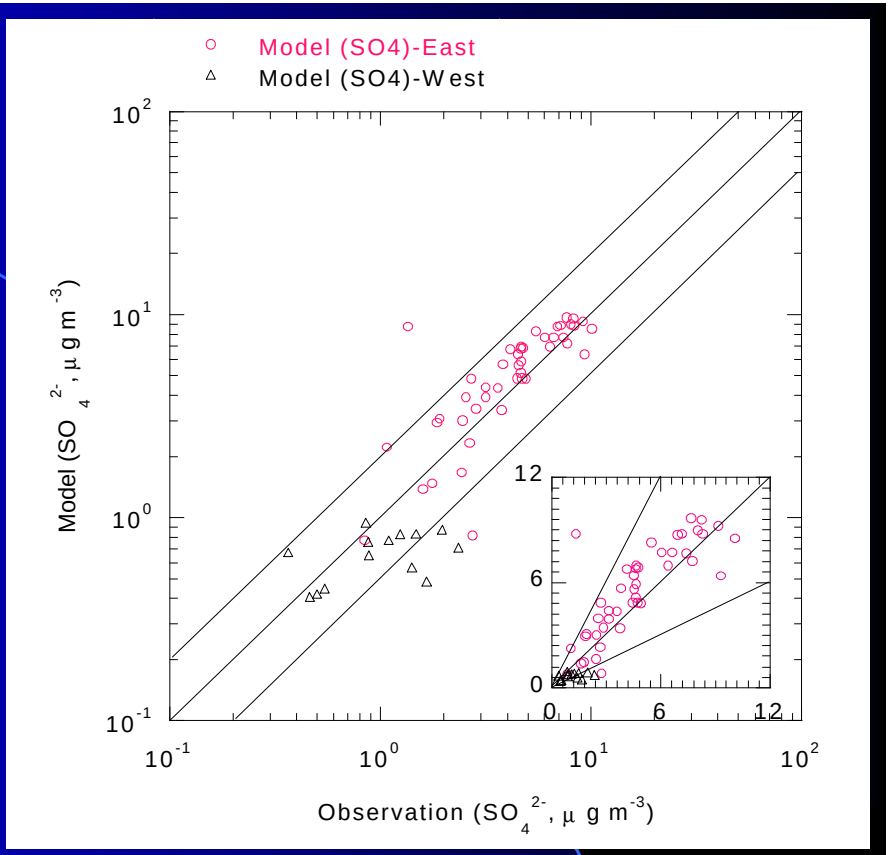


CMAQ Performance

- Most simulations within 2:1
- Biases are positive and small
- Errors are also small
- Results better in eastern US

SO_4

- Week mean
- CASTNet



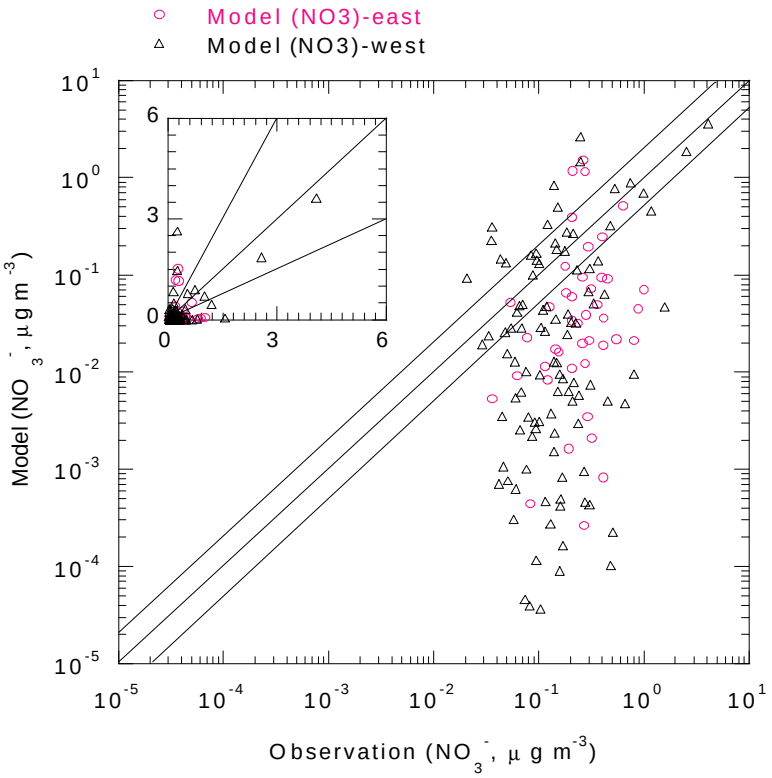
	CMAQ	OBS	CMAQ = 0.46 + 1.03 OBS	
Mean	4.42	3.85	n	59
SD	3.10	2.64	R	0.88
CV	70.1%	68.7%	MB	0.57
Max	9.70	10.10	MNB	17.8%
95th	9.24	9.15	MFB	3.5%
75th	6.97	5.47	MAGE	1.11
50th	4.37	3.16	MNGE	40.3%
25th	0.87	1.59	NME	28.8%
5th	0.47	0.50	NMB	15.1%
Min	0.41	0.36	RMSE	1.58

CMAQ Performance

- Most simulations within 2:1
- Biases still positive and small
- Errors still small
- Results better in eastern US

NO_3

- 24-Hr mean
- IMPROVE



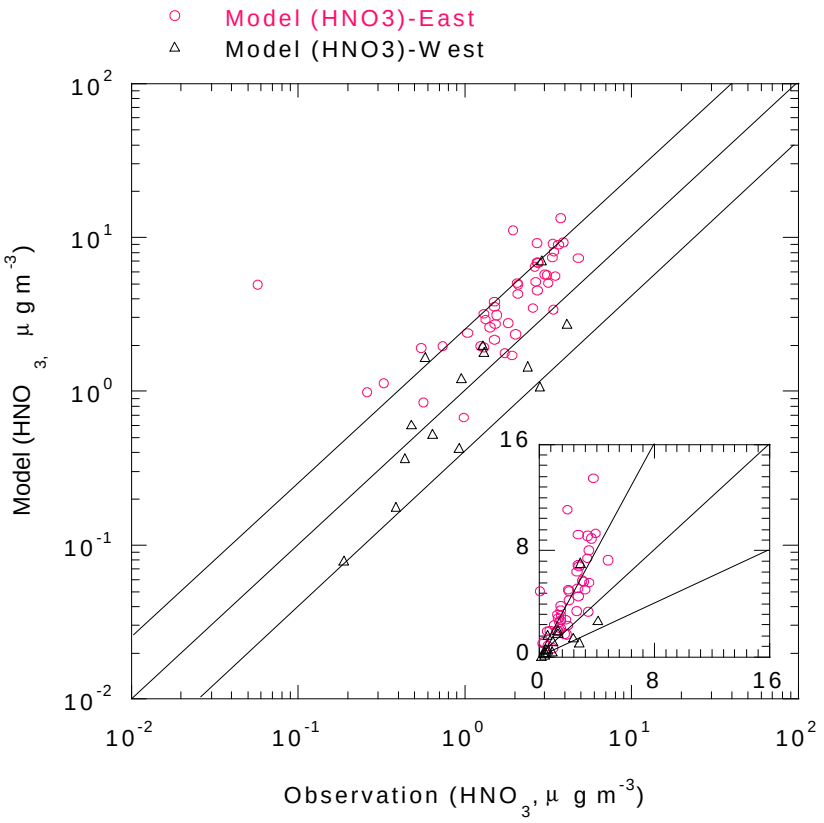
	CMAQ	OBS	CMAQ = -0.02+ 0.68 OBS	
Mean	0.17	0.28	n	147
SD	0.46	0.44	R	0.64
CV	271.5%	157.9%	MB	-0.11
Max	3.62	4.08	MNB	-24.7%
95th	0.89	0.81	MFB	-108.3%
75th	0.10	0.29	MAGE	0.24
50th	0.02	0.17	MNGE	109.7%
25th	0.0	0.09	NME	85.4%
5th	0.0	0.04	NMB	-39.3%
Min	0.0	0.02	RMSE	0.39

CMAQ Performance

- Biases are negative and large
- Errors are also large
- Few simulations within 2:1

HNO_3

- Week mean
- CASTNet



	CMAQ	OBS	CMAQ = 0.22 + 1.88 OBS	
Mean	3.89	1.95	n	59
SD	3.02	1.16	R	0.72
CV	77.6%	59.7%	MB	1.94
Max	13.40	4.79	MNB	234.3%
95th	9.31	3.91	MFB	49.2%
75th	5.69	2.81	MAGE	2.13
50th	2.92	1.82	MNGE	247.0%
25th	1.72	0.98	NME	109.2%
5th	0.37	0.26	NMB	99.5%
Min	0.08	0.06	RMSE	3.01

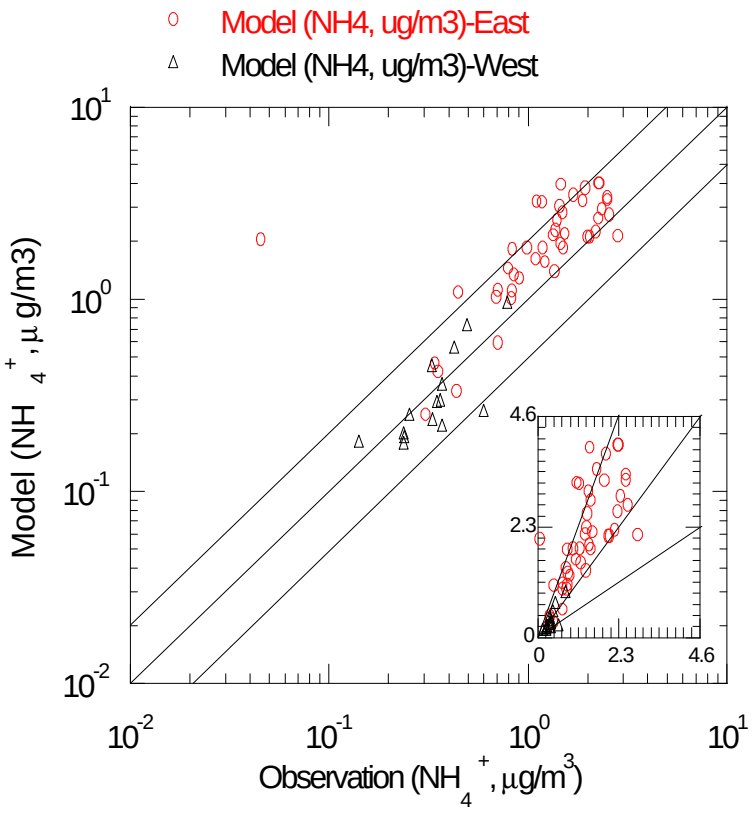
CMAQ Performance

- Most simulations within 2:1
- Biases positive and large
- MNB, MNGE inflated due to small observed concentrations

NH_4

- Week mean
- CASTNet

	CMAQ	OBS	CMAQ = 0.22 + 1.31 OBS	
Mean	1.68	1.12	n	59
SD	1.20	0.75	R	0.82
CV	71.0%	67.5%	MB	0.57
Max	4.03	2.83	MNB	114.1%
95th	3.90	2.50	MFB	28.7%
75th	2.62	1.52	MAGE	0.63
50th	1.60	0.94	MNGE	124.1%
25th	0.46	0.40	NME	56.3%
5th	0.20	0.24	NMB	50.9%
Min	0.18	0.05	RMSE	0.91



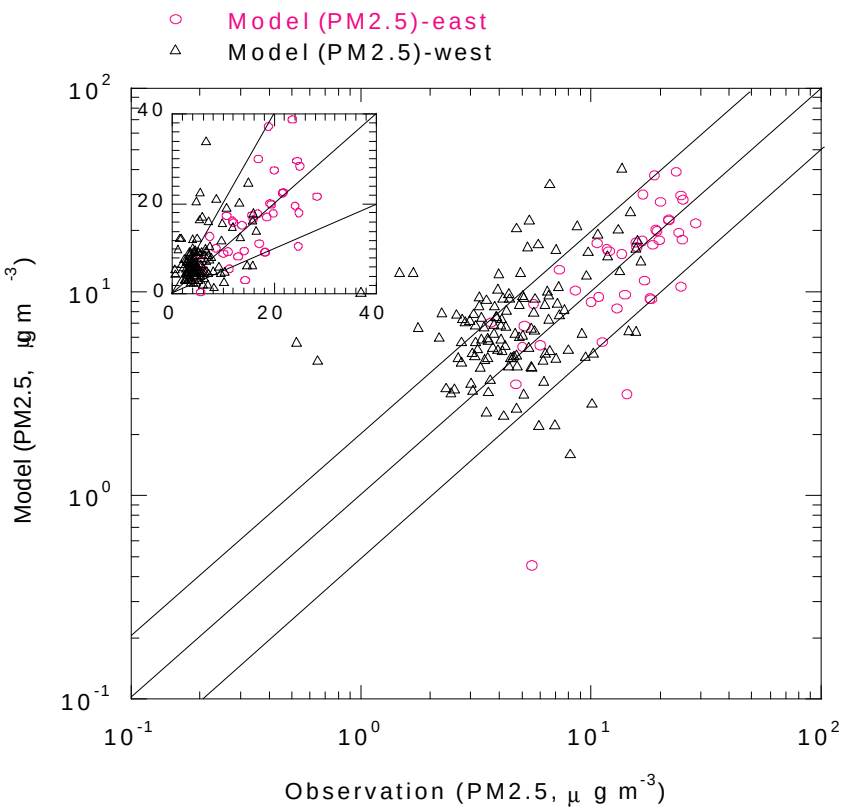
CMAQ Performance

- Almost all simulations within 2:1
- Biases are positive and large
- Errors are also large

$PM_{2.5}$

- 24-Hr mean
- IMPROVE

	CMAQ	OBS	CMAQ = 3.70 + 0.81 OBS	
Mean	10.12	7.95	n	164
SD	7.51	6.15	R	0.66
CV	74.2%	77.3%	MB	2.17
Max	40.70	28.50	MNB	68.8%
95th	24.90	21.70	MFB	25.3%
75th	12.50	10.70	MAGE	4.25
50th	7.58	5.40	MNGE	87.8%
25th	5.17	3.71	NME	53.5%
5th	3.15	2.35	NMB	27.3%
Min	0.45	0.53	RMSE	6.13



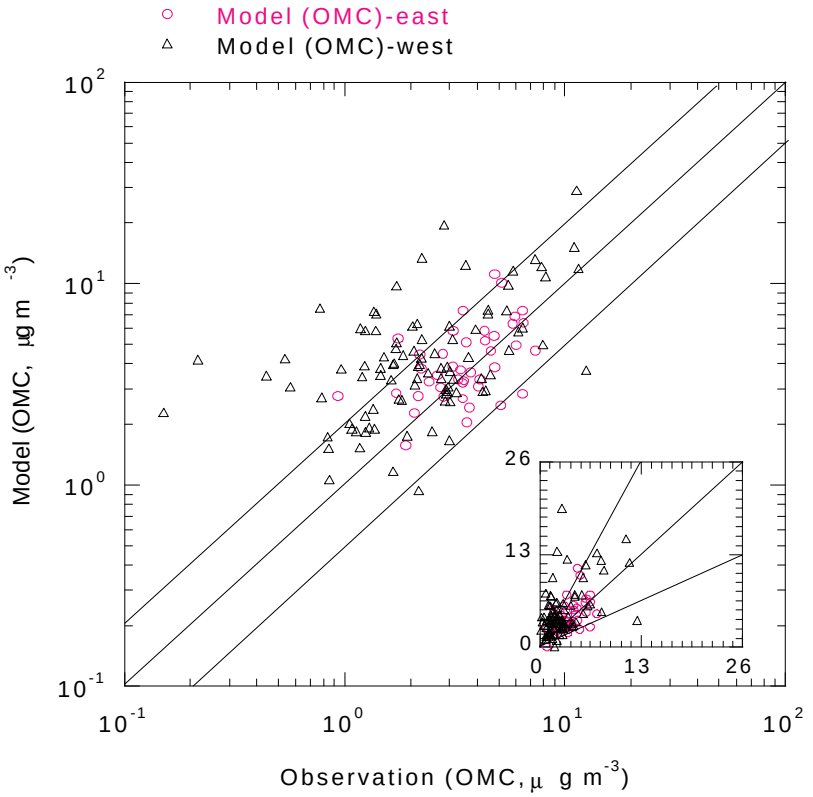
CMAQ Performance

- Most simulations within 2:1
- Biases are positive and large
- Errors are also large

OMC

- 24-Hr mean
- IMPROVE

	CMAQ	OBS	CMAQ = 1.97 + 0.89 OBS	
Mean	4.81	3.20	n	138
SD	3.71	2.29	R	0.55
CV	77.0%	71.5%	MB	1.61
Max	29.10	12.50	MNB	112.8%
95th	12.20	7.85	MFB	37.1%
75th	5.81	4.18	MAGE	2.23
50th	3.80	2.74	MNGE	127.2%
25th	2.83	1.66	NME	97.4%
5th	1.53	0.79	NMB	70.3%
Min	0.03	0.15	RMSE	3.49

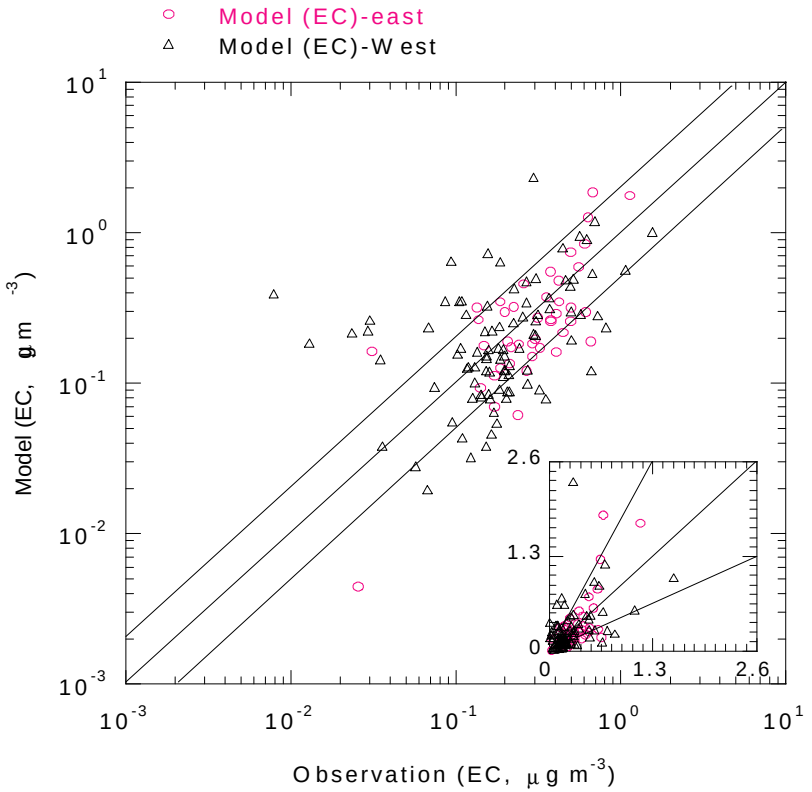


CMAQ Performance

- Majority simulations within 2:1
- Biases are positive and large
- Errors are also rather large`

EC

- 24-Hr mean
- IMPROVE



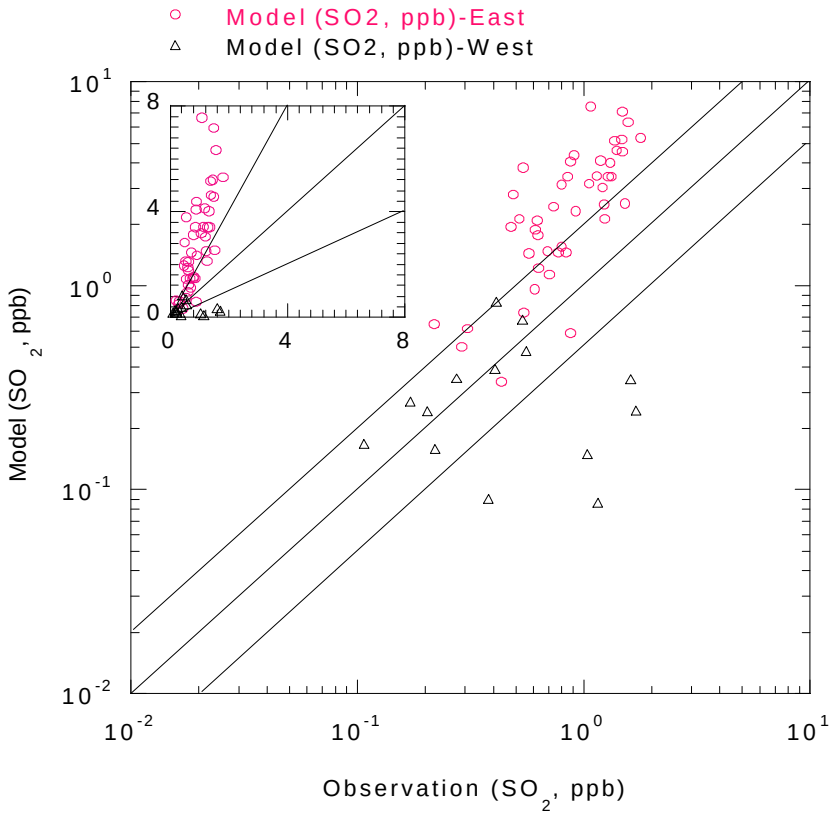
	CMAQ	OBS	CMAQ = 0.07 + 0.81 OBS	
Mean	0.31	0.29	n	136
SD	0.34	0.23	R	0.54
CV	112.8%	81.1%	MB	0.02
Max	2.33	1.56	MNB	80.0%
95th	0.96	0.67	MFB	-7.0%
75th	0.34	0.37	MAGE	0.17
50th	0.19	0.21	MNGE	128.6%
25th	0.12	0.15	NME	58.6%
5th	0.04	0.03	NMB	-6.6%
Min	0.00	0.01	RMSE	0.29

CMAQ Performance

- Majority simulations within 2:1
- Biases are small and mixed
- Errors are large

SO_2

- Week mean
- CASTNet



	CMAQ	OBS	CMAQ = -0.02 + 2.66 OBS	
Mean	2.24	0.85	n	59
SD	1.89	0.44	R	0.63
CV	84.4%	52.4%	MB	1.40
Max	7.56	1.78	MNB	152.4%
95th	6.33	1.61	MFB	58.5%
75th	3.42	1.23	MAGE	1.58
50th	1.88	0.80	MNGE	170.0%
25th	0.59	0.52	NME	185.9%
5th	0.15	0.20	NMB	164.7%
Min	0.09	0.11	RMSE	2.15

CMAQ Performance

- Biases are positive and very large
- Errors are also very large

Evaluation Summary

	n	r	MB	MNB %	MFB %	MAGE	MNGE %	NME %	NMB %	RMSE
O_3 Hourly	234,384	0.68	10.8	111.0	31.4	15.2	122.4	31.4	23.7	19.5
O_3 Max 1- hr	10,149	0.71	9.2	22.7	16.4	14.0	29.0	24.0	15.8	18.0
O_3 Max 8- hr	10,149	0.72	10.4	29.1	21.1	13.2	33.6	26.9	21.2	16.5
SO_4 CASTNet	59	0.88	0.57	17.8	3.5	1.11	40.3	28.8	15.1	1.58
SO_4 IMPROVE	174	0.92	0.19	32.6	2.1	0.73	61.0	36.8	9.5	1.31
NO_3	147	0.64	-0.11	-24.7	-108.3	0.24	109.7	85.4	-39.3	0.39
$PM_{2.5}$	164	0.66	2.17	68.8	25.3	4.25	87.8	53.5	27.3	6.13
NH_4	59	0.82	0.57	114.1	28.7	0.63	124.1	56.3	50.9	0.91
SO_2	59	0.63	1.40	152.4	58.5	1.58	170.0	185.9	164.7	2.15
HNO_3	59	0.72	1.94	234.3	49.2	2.13	247.0	109.2	99.5	3.01
OMC	138	0.55	1.61	112.8	37.1	2.23	127.2	97.4	70.3	3.49
EC	136	0.54	0.02	80.0	-7.0	0.17	128.6	58.6	- 6.6	0.29

Evaluation Summary

CMAQ

- varies in its ability to simulated air concentrations of the nine species
  - correlations range from ~ 0.55 (EC, OMC) to ~ 0.90 (SO_4)
  - NME range from ~ 25% (O_3) to over 100% (HNO_3, SO_2)
- generally over-predicts
  - biases are positive (except NO_3, EC) and for some species large
- performs better for O_3 and SO_4 than other species

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